

Chlorbromuron
13360-45-7 | DTXSID6040290

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 321 °C

Global applicability domain: Inside

Local applicability domain index: 2.68e-01

Confidence level: 5.85e-01

Nearest Neighbors from the Training Set

Image not found

3-Nitrobenzamide

Measured: 313

Predicted: 310

Image not found

2-Nitrobenzamide

Measured: 317

Predicted: 310

Image not found

Benzoic acid, 2-phenylhydrazide

Measured: 314

Predicted: 306

Image not found

Propanil

Measured: 351

Predicted: 317

Image not found

N-Butylbenzenesulfonamide

Measured: 314

Predicted: 286